A Computational Workbench Environment for Virtual Power Plant Simulation

Quarterly Progress Report

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Abstract

This is the eighth Quarterly Technical Report for DOE Cooperative Agreement No: DE-FC26-00NT41047. The goal of the project is to develop and demonstrate a computational workbench for simulating the performance of Vision 21 Power Plant Systems. Within the last quarter, good progress has been made on all aspects of the project. Calculations for a full Vision 21 plant configuration have been performed for two coal types and two gasifier types. Good agreement with DOE computed values has been obtained for the Vision 21 configuration under "baseline" conditions. Additional model verification has been performed for the flowing slag model that has been implemented into the CFD based gasifier model. Comparisons for the slag, wall and syngas conditions predicted by our model versus values from predictive models that have been published by other researchers show good agreement. The software infrastructure of the Vision 21 workbench has been modified to use a recently released, upgraded version of SCIRun.

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Executive Summary

The work to be conducted in this project received funding from the Department of Energy under Cooperative Agreement No: DE-FC26-00NT41047. This project has a period of performance that started on October 1, 2000 and continues through September 30, 2003.

The goal of the project is to develop and demonstrate a computational workbench for simulating the performance of Vision 21 Power Plant Systems. The Year One effort focused on developing a *prototype workbench* for the DOE Low-Emissions Boiler System (LEBS) Proof of Concept (POC) design. The Year Two effort is focused on developing a more advanced workbench environment for simulating a gasifier-based Vision 21 energyplex.

The main accomplishments during the last three months include:

- A fully functional version of the Vision 21 workbench has been completed. A complete set of models for the Vision 21 configuration provided by DOE have been developed and implemented into the workbench. Calculations for the full plant configuration have been performed for two coal types and two gasifier types. Good agreement with DOE computed values has been obtained for the Vision 21 configuration under “baseline” conditions.
- Model verification has been performed for the flowing slag model that has been implemented into the CFD based gasifier model. Comparisons for the slag, wall and syngas conditions predicted by our model versus values from predictive models that have been published by other researchers show good agreement.
- The software infrastructure of the IGCC workbench has been modified to use a recently released, upgraded version of SCIRun.
- Preliminary work has been performed for developing a standardized model interface, tailored to Vision 21, using the SIDL interface definition language. This standard interface will be used to create interoperability of CCA components.

Each of these topics is discussed in the following sections.

Experimental Methods

Within this section we present brief discussions on the many sub-tasks that must be addressed in developing the workbench. For simplicity, the discussion items are presented in the order of the Tasks as outlined in our detailed Work Plan.

Task 1 – Program Management

A podium presentation that highlighted material from this project was made at the Gasification Technologies Conference 2002, held October 28-30, 2002 in San Francisco, California [Bockelie et al, 2002e]. The paper, entitled "CFD Modeling for Entrained Flow Gasifiers", highlighted the CFD modeling capability for entrained flow gasifiers that has been created within this project. Included in the paper is an overview of our CFD model and results for parametric simulations.

On October 8, 2002 project team members visited the DOE Albany Research Center (ALRC) in Albany, Oregon. The refractory group at ALRC has a DOE funded project to increase the life of refractory used in gasifiers. Discussions focused on technical information exchanges based on our respective current projects, areas of potential collaboration and possible future projects.

On November 19-20, 2002 project team members attended a Vision 21 Simulation Workshop held at the Iowa State University Virtual Reality Applications Center (VRAC) in Ames, Iowa. At the meeting a podium presentation was provided entitled "A Computational Workbench Environment for Vision 21 Energyplex Simulation" that highlighted modeling results of our Vision 21 reference configuration (see results section of this report). As part of the meeting, CFD results for the one and two stage gasifier models were presented using the VRAC C4, four walled, immersive environment.

On November 19-20, 2002 project team members attended the Fuel Cell Seminar and Workshop hosted by the National Fuel Cell Research Center, held in Palm Springs, California, USA.

On December 9, 2002 project team members met with Neville Holt (EPRI), a consultant to this project. The meeting provided us the opportunity to discuss our progress on developing entrained flow gasifiers models and to discuss publicly available data for use in model development and verification.

An abstract for a paper entitled "A Process Workbench for Virtual Simulation of Vision 21 Energyplex Systems" has been accepted for presentation at the 28th International Technical Conference on Coal Utilization & Fuel Systems, to be held March 10-13, 2002 in Clearwater, Florida, USA [Bockelie et al, 2003]. The paper will highlight recent model results obtained with our IGCC workbench.

Task 2 – Virtual Plant Workbench II

The objective of this task is to further develop the capabilities of the computational workbench environment with the goal of providing the infrastructure needed to model a Vision 21 energyplex system. For the many sub-tasks contained under Task 2, the work effort is being performed by software engineers from Reaction Engineering International (REI) and Visual Influence (VI).

The main focus of this sub-task has been to continue to evolve a comprehensive software design, building on the ideas developed for Workbench I. As the complexity and capabilities of Workbench II continue to increase, the software design is evaluated and modified accordingly.

Component Interfaces

During the last performance period, we have continued to focus our efforts on utilizing component architecture methodologies to interface models to the workbench. We persist in believing this is a vital aspect of the software design. This belief is routinely reinforced as we see component architectures continue to gain momentum as the future of computing and software engineering.

As noted previously on numerous occasions, proper model integration techniques can provide significant advantages, most notably model interoperability among the various Vision 21 teams and third-party developers. For the Year One prototype workbench (Workbench I), model integration was performed using C++ wrapper classes to encapsulate the model of interest; this is a proven, traditional method of integrating models into SCIRun and other problem solving environments. For the Vision 21 Energyplex workbench (Workbench II), we have implemented a more sophisticated approach based on component architecture methods for software integration.

Workbench II Model Integration Paradigm: To address the functional requirements of Workbench II, model integration techniques have been extended to include the use of component architectures with standardized interfaces. Component architectures alone offer numerous advantages when compared with conventional programming techniques. These advantages include programming language and platform independence, location transparency (and hence parallelism) and reuse. When these core advantages of component architectures are coupled with standardized interfaces, reuse becomes interoperability.

For Workbench II, we have created the necessary infrastructure to support two different component architecture standards: CCA and CORBA. These component architectures are discussed in additional detail in the following paragraphs.

CCA (Common Component Architecture) was created to address the need for a component architecture for HPC [http://www.acl.lanl.gov/cca-forum/]. The creation of the CCA forum, which oversees the development of the CCA standard, was inspired by the DOE2000 initiative. The specification created by this group provides the benefits of the standard business oriented component architectures (interoperability, language independence, parallel capabilities), while addressing the issues of high-performance computing such as parallel communication channels between components and other elements required for dealing with extremely large data sets.

CORBA is a widely used, business-oriented component architecture standard developed by the Object Management Group (OMG). The OMG is an open membership, not-for-profit consortium that produces and maintains computer industry specifications for interoperable enterprise applications. Membership includes virtually every large company in the computer industry, and hundreds of smaller ones. While lacking in the high performance features of the CCA, the wide user base of CORBA makes it a logical choice for small-to-medium sized computational models.

As noted above, one of the key advantages of using component architectures with standard interfaces is interoperability. For Workbench II, the standard interfaces being used are 1) CAPE-OPEN for CORBA and 2) V21_CCA for CCA.

CAPE-OPEN [http://www.colan.org] is a set of standards created to facilitate the use of COM and CORBA component software for process engineering problems. This standard has been well received by the process engineering community. By enabling support for CAPE-compliant components in Workbench II, we gain access to a potentially large number of process engineering models.

V21_CCA is a set of standards being developed by REI and VI software engineers specifically to address the need for interoperability of computational models developed for the Vision 21 program. It is anticipated that other Vision 21 teams developing software will make use of this open standard such that interoperability between teams becomes a reality. We anticipate a DRAFT version of these standards to be available for review by the end of the next quarter.

By providing functionality in Workbench II for both prevailing component architectures and their corresponding standards, we believe we have created a highly versatile software environment that provides a high level of flexibility to handle computational models from many sources and with diverse implementations.

Enhancements to the SCIRun Framework - Updated SCIRun:

Recently, the University of Utah Scientific Computing and Imaging Institute (SCI) released version 1.8 of SCIRun. As we desire to keep pace with the latest developments made by the University of Utah's SCI group, we have upgraded all workbench models and their interfaces to comply with this newest SCIRun. Simplified installation, improved visualization and expanded error handling are all benefits realized by this upgrade.

Task 2.2 Visualization

As stated in previous reports, a link has been created between SCIRun and OpenDX to give the workbench user access to the large range of visualization and data analysis capabilities provided by OpenDX. During the last performance period, a new effort has been undertaken to further extend the visualization capabilities of the workbench by adding Virtual Reality (VR) capabilities. The goal of these efforts will be to enable the user to visualize complex data sets in a myriad of ways on a full range of visualization hardware, from a simple CRT all the way to a multi-walled, immersive environment.

The VR capability is being implemented using several pre-existing software toolkits. For core scientific visualization calculation functionality, the Visualization Tool Kit (VTK) [http://www.vtk.org/] is being used. VTK is an extensive class library which supports a full range of scientific visualization operations. Using VTK as only a calculation engine, we take VTK "actor" objects and pass them through vtkActorToPF [http://brighton.ncsa.uiuc.edu/~prajlich/vtkActorToPF/], which is a small library that converts the information generated by VTK to SGI's OpenGL Performer. Once the information regarding the visualization exists as a Performer scenegraph, we are able to make use of vrJuggler [http://www.vrjuggler.org/] to handle calculations related to hardware abstraction.

Task 2.3 Module Implementation/Integration

The focus of this sub-task has been to continue the development of component wrappers needed for Workbench II computational components and to start integrating into the workbench component modules for equipment downstream.

Component Model Integration:

Having the required complement of modules needed to model a complete system, this past performance period we have focused on performing large network simulations and debugging all aspects of the workbench.

Task 2.4 Vision 21 Demonstration

As discussed in the results section below, there is good agreement between performance parameters provided by DOE for the Vision 21 reference configuration and those generated by the workbench. A by-product of modeling the reference configuration has been to exercise the functionality of the workbench. Overall, we have been quite pleased with the versatility of the workbench. We have demonstrated a "plug and play" functionality – models can be deleted or added as needed. In addition, the use of component architecture software techniques provides for a mechanism to allow models to be re-used across different modeling systems.

Task 3 – Model Vision 21 Components

The purpose of this task is to develop the reactor and CFD models for the components that will be included in the workbench. In general, these models are first developed in a “stand-alone” form and then subsequently integrated into the workbench environment.

<u>Vision 21 Energy Plex Configuration</u>
Illustrated in Figure 1 is the Vision 21 energyplex configuration that the DOE Vision 21 Program Manager has suggested be used by this project to demonstrate the capabilities of our workbench environment. This configuration consists of an entrained flow gasifier, gas clean up system, gas turbines, heat recovery steam generator, steam turbine and SOFC fuel cells. As described below, a combination of CFD and reactor models will be used to simulate the performance of this configuration. A CFD model will be used for the entrained flow gasifier and simpler models will be used for the remainder of the equipment and processes.

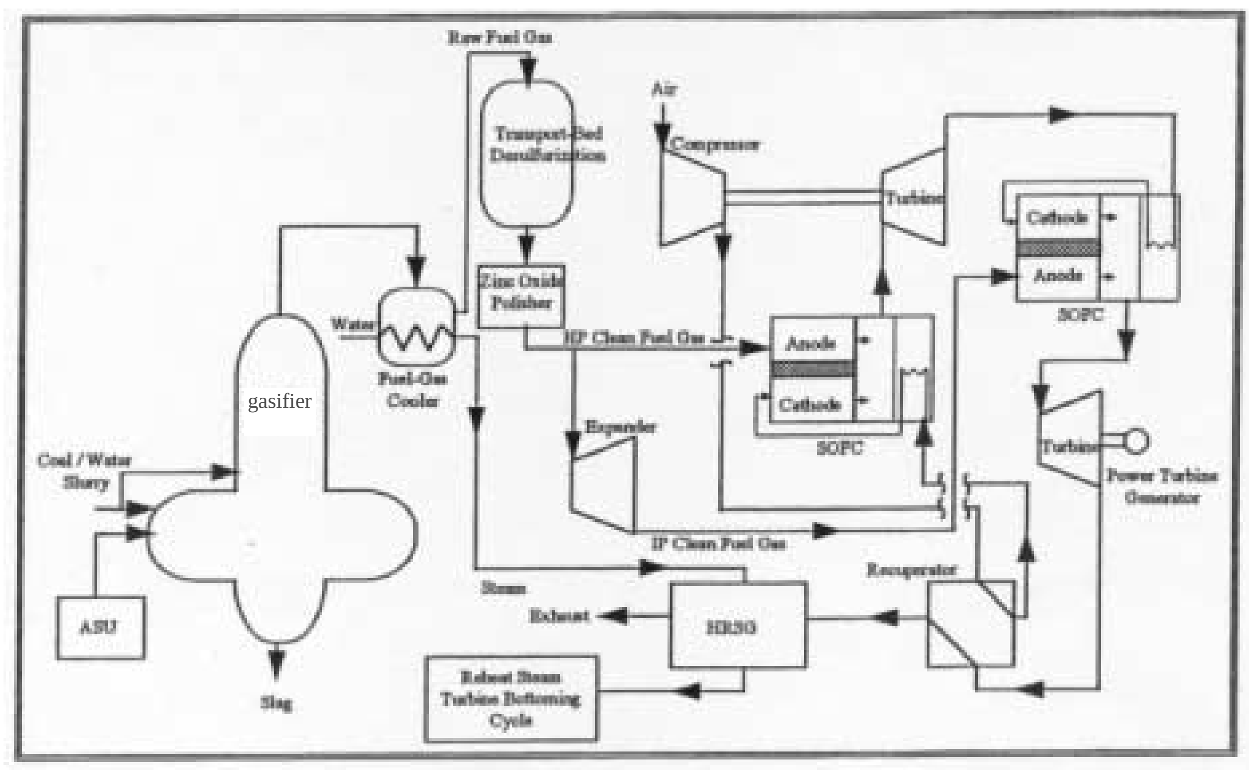


Figure 1. DOE selected Vision 21 test case configuration.

Listed in Tables 1 and 2 are the gross conditions for the configuration that were originally provided by DOE. Shown in Figure 2 is a mass and energy balance sheet obtained from DOE that provides more detailed information about the targeted Vision 21 configuration. A comparison of Figures 1 and 2 shows some discrepancies. As noted in previous progress reports, where information is missing we have used data available in the literature, combined with engineering judgment, to develop the required information to create the needed models.

Table 1. Provided Operating Conditions for Vision 21 Energyplex

Gasifier (18 atm)	Two-stage, up-fired
Coal Input to Gasifier (lb/hr)	256,142
Coal Type	Illinois #6
Thermal Input (MW)	875.8
HP SOFC dc/ac	189.4/182.8
LP SOFC dc/ac	121.4/117.2
Gas Turbine, MW	133.7
Steam Turbine, MW	118.0
Fuel Expander, MW	9.6
Gross Power	561.3
Auxiliary Power, MW	40.4
Net Power, MW	520.9
Efficiency, % HHV	59.5

Table 2. Illinois Coal #6 Description

Proximate Analysis	As-Received (wt%)
Moisture	11.12
Ash	9.70
Volatile Matter	34.99
Fixed Carbon	44.19
TOTAL	100.00
HHV (Btu/lb)	11666
Ultimate Analysis	As-Received (wt%)
Moisture	11.12
Carbon	63.75
Hydrogen	4.50
Nitrogen	1.25
Sulfur	2.80
Ash	9.70
Oxygen (by difference)	6.88
TOTAL	100.00

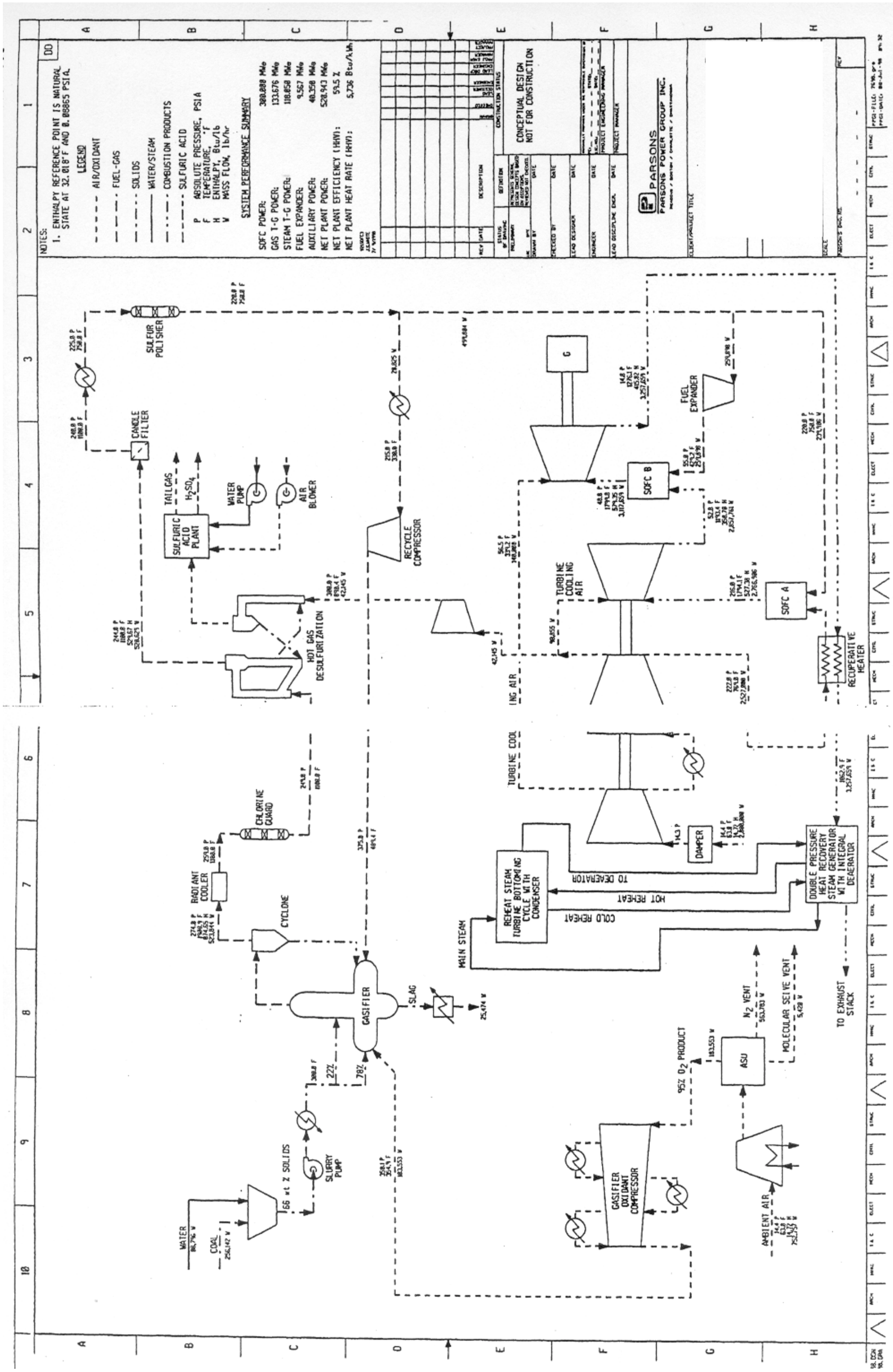
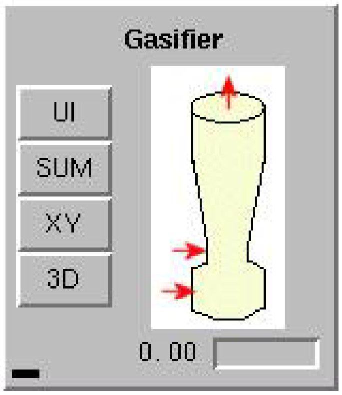


Figure 2. Mass and Energy Balance sheet provided by DOE for Vision 21 reference configuration.

Task 3.3 Gasifier Models

Good progress has been made on developing CFD based models for entrained flow gasifiers. The models are being created using two different CFD codes. REI personnel will develop one gasifier model with *GLACIER* - a comprehensive two-phase CFD based reacting CFD code. At present, *GLACIER* is limited to performing steady-state simulations and thus will be used to perform steady state CFD simulations of single and two-stage gasifiers. The other gasifier model will be developed by RECOM using *AIOLOS*, a comprehensive reacting CFD code capable of performing transient boiler simulations and thus will be used to perform time dependent simulations for a single stage gasifier. Both CFD codes have been used to analyze numerous coal-fired industrial combustion systems. The two codes employ different meshing technologies and different assumptions and sub-models for turbulence-chemistry interaction, simulating two-phase flow and reaction kinetics for combustion and gasification.

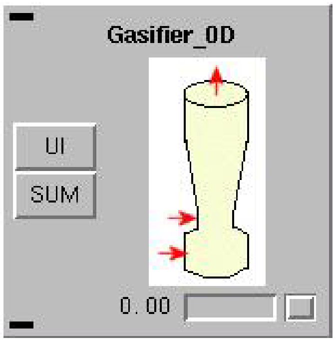
Below we highlight the progress within the last performance period in developing the CFD based gasifier models.



***GLACIER* Gasifier Module (Steady State)**:. During the last performance period, our efforts for this model have focused on completion of a 0D pre-processor gasifier model and performing simulations to allow comparing our model results versus previous DOE NETL reported values for Vision 21 conditions. Details about the model development are described immediately below, whereas further details on the CFD and system results are described in the Results and Discussion Section of this report.

0-D Gasifier Model

The CFD gasifier model requires significant computational time to arrive at a steady-state solution. Hence, there is a need for a simpler model that may be used for faster calculations either within the energyplex workbench or as a preprocessor to optimize operating inputs before running the CFD model. The model can be used to optimize gasifier efficiency while providing indicators for proper slag flow. During the last performance period this model was extended to handle a two-stage gasifier.



The 0-D gasifier model consists of two submodels: an equilibrium zonal equilibrium submodel with heat transfer and a coal burnout submodel. The zonal submodel calculates the equilibrium exit gas concentration and temperature given a prescribed heat transfer through the walls. An ash viscosity submodel from the CFD gasifier slag model is used to calculate a representative ash viscosity and critical viscosity temperature. The fuel burnout and char recycle are required inputs to the zonal submodel obtained from the burnout submodel, while the gas and radiation temperatures are the required inputs into the burnout submodel obtained from the zonal submodel. A schematic of the 0D model for a one and two stage gasifier are illustrated in Figures 3a and 3b, respectively.

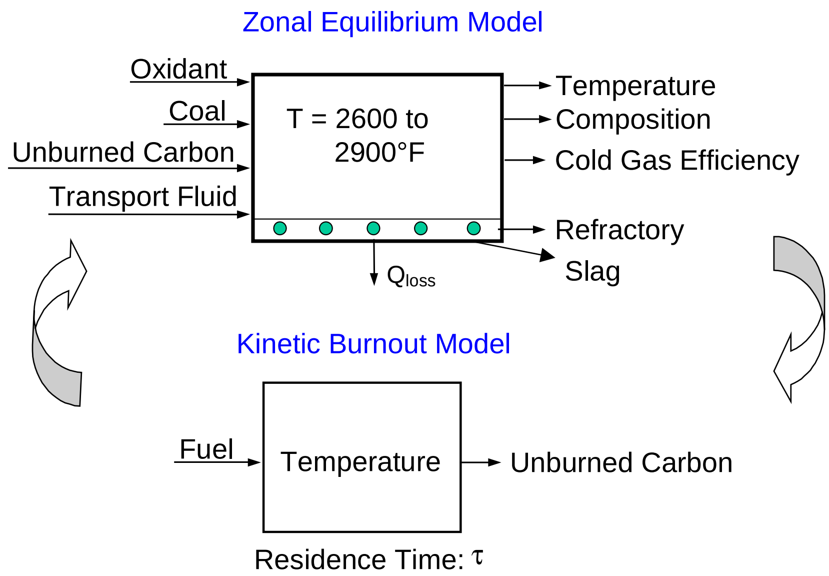


Figure 3a. Schematic for the one stage, 0-D gasifier pre-processor model.

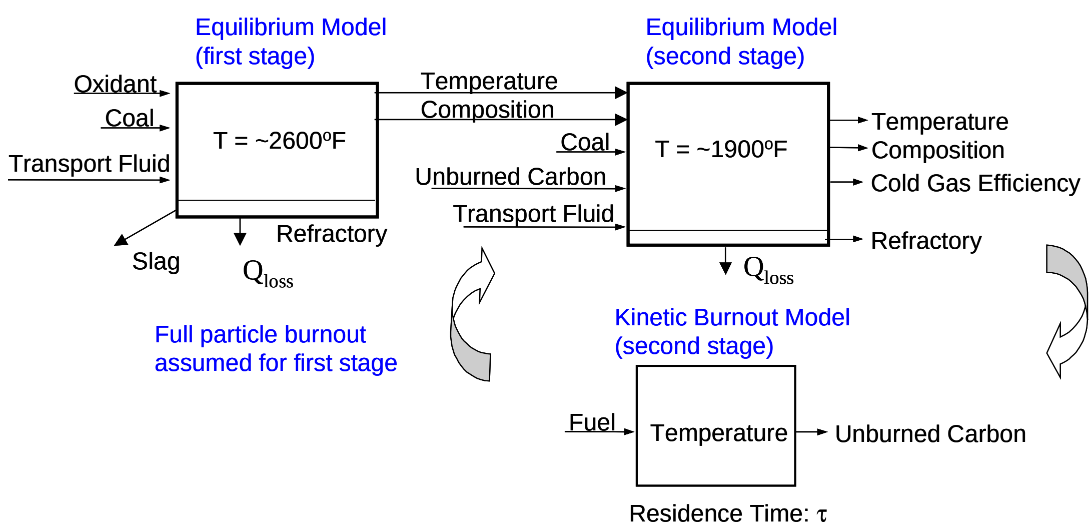


Figure 3b. Schematic for the two-stage, 0-D gasifier model.

For particle burnout we have used CBK8, a model developed at Brown University [Sun and Hurt, 2000] which includes intrinsic oxidation of coal in lean pulverized combustion. High-pressure heterogeneous gasification reactions under substoichiometric conditions have been incorporated as global rates. However, we are looking at an in-house heterogeneous particle reaction model, which is extensible to use other kinetic data that we anticipate will be become available from the Collaborative Research Center for Coal and Sustainable Development (CCSD) in Australia.

During the last performance period, we have completed the extension of the 0D gasifier model involving CBK8 to handle two-stage gasifiers. This was accomplished by essentially coupling two one-stage gasifier models with the outlet of the first acting as an inlet for the second along with additional inlet flows representing the staged fuel and transport fluid (see Figure 3b). Two-stage gasifiers are operated with the first stage serving as a combustion stage, which provides the heat needed to drive endothermic gasification reactions in the reducing second stage. The first stage is operated closer to stoichiometric, while the remaining feed-stock fuel is introduced in the second stage with very little or no oxidant. Therefore, the fuel injected in the first stage usually has complete burnout. In the present two-stage model complete burnout in the first stage is assumed and no burnout calculations are performed for that stage. This assumption has been necessary with the use of CBK8, which was not written to accommodate staged fuel injection. A significant rewrite of CBK8 would be required to introduce partially burned char in the second stage. By using an in-house heterogeneous particle reaction model, we will be able to relax the burnout assumption of the first stage.

Task 3.4 Gas Cleanup and other equipment models

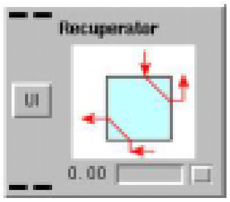
In this sub-task we will develop many of the modules required to simulate the Vision 21 energyplex system. This will include models for the:

- Syngas Cooler
- Heat Recovery Steam Generator
- Gas Recuperator
- SCR
- Turbines, compressors and expanders
- Cyclone separator
- Gas Clean Up
- High and Low Pressure Solid Oxide Fuel Cell

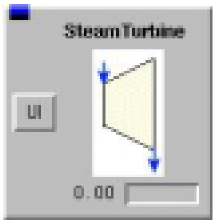
These systems are modeled with 0D, or at most 1D, reactor models. Many of these models have been created by re-using models developed as part of the LEBS-POC prototype workbench developed during Year One of the program. Details on the models used in the Year One prototype workbench are available in [Bockelie et al, 2001], [Bockelie et al, 2002a].

All of the required models have been developed, tested and implemented into our IGCC workbench. Future work on these models will focus on refining the assumptions within a model when results indicate a need.

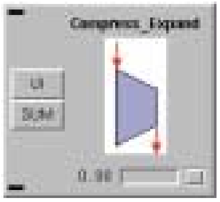
In the following, we provide a brief, self contained description of each component model. For detailed descriptions of the models, see [Bockelie et al, 2002b,d].



Recuperator. The recuperator is a gas-to-gas heat exchanger used to preheat the compressed air being fed to the high pressure SOFC. A 0D model has been developed based on the 0D air preheat heat exchanger model developed for the Year One prototype workbench. As per the other heat exchanger models, the recuperator model has been sized for the specified gas temperatures provided by the DOE.



Steam Turbines. A simple 0D steam turbine model based on thermodynamic calculations using a user input adiabatic efficiency has been implemented. The efficiency is applied to an isentropic expansion process using the ASME 67 steam properties module.

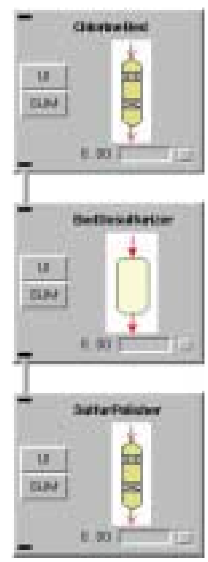


Compressor/Expander: Compressor and expander components are modeled with a simple 0D model. The thermodynamic calculations involve the assumption of an isentropic compression/expansion processes, coupled with user supplied isentropic efficiencies. The thermodynamic properties needed for these models are obtained using a thermodynamics database class contained within the workbench that can be accessed by any module as needed.

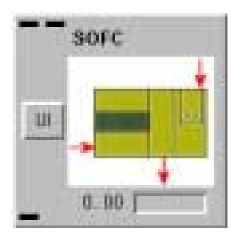
Gas Turbine Combustor: At present, the gas turbine combustor is module consists of a 0D chemical equilibrium-based model. In future work we will investigate the possibility of using alternative models and potentially catalytic combustors.

Cyclone Separator: In the DOE Vision 21 reference configuration a cyclone particle separator is located immediately downstream of the gasifier and serves the purpose of eliminating particulate matter from the syngas before it reaches the gas clean up system. This 0D model makes use of mathematical correlations to calculate pressure drop and particulate removal efficiency as a function of particle diameter [De Nevers, 2000]. Required gas phase thermodynamic properties are obtained from a thermodynamics database class within the workbench.

Gas Clean Up. The Vision 21 reference configuration originally was to use hot gas clean up (~1000F). However, based on advice from the DOE, we currently are targeting warm gas clean up (500-900F). At present there is little, if any, operating experience for full scale equipment in either temperature regime. Hence, the gas clean up system is modeled with a sequence of simple, 0D reactor models. The equipment and process components are appropriate for both hot and warm gas clean up processes. The equipment components in the train include a chlorine bed guard for HCl removal and a transport reactor desulfurizer and sulfur polisher for removal of H_2S, and COS. For these models, the user must specify the removal efficiency (%) and temperature change (loss) across each component. We have implicitly assumed that HCl, H_2S and COS are the main pollutants that need to be removed. The pressure drop across the components can be calculated or specified by the user. The performance of sorbents used for the gas clean up is not included in the models. Default values are provided for all model inputs.



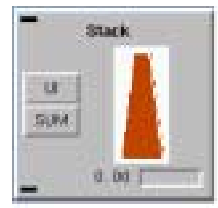
High and Low Pressure Fuel Cell Models: A lumped parameter, 0D model and a transient 1D model to describe the performance of solid oxide fuel cells were obtained from DOE-NETL. Brief descriptions of the implemented models are provided below. For more detailed descriptions see [Bessette, 1994], [Gemmen et al, 2000], [Liese and Gemmen, 2002], [Liese et al, 2000].



0D Fuel Cell Model: The model makes use of the Nernst equation and equations for activation, concentration and ohmic losses to calculate fuel cell electrical output. Thermodynamics calculations are performed using a combination of equilibrium and heat exchanger cacluations. The anode temperature is iterated until the thermodynamic output from the fuel cell matches the electrical output. The model obtained from DOE-NETL was developed for use in Aspen-Plus and employed a combination of Aspen-Plus functions and imbedded FORTRAN. The DOE model was subsequently re-implemented using C++ for use in the workbench. Enhancements from the NETL fuel cell model include the ability to use coal derived syngas as the fuel gas, operation at elevated pressure, removal of the fuel gas reformer (not needed for IGCC) and more robust equation solvers.

1D Fuel Cell Model: The 1D fuel cell model obtained from DOE-NETL is implemented in C++ and is much more sophisticated than the 0D model [Gemmen et al, 2000]. The model accounts for energy transport in and out of a flow channel of a fuel cell, heat transfer to and from the walls, heat generation from the electrochemical reactions and fuel cell power output. A finite difference approach is used to solve the mass, momentum and energy conservation equations. The model uses a dynamic simulation approach that is geared for performing the safety analysis of hybrid fuel cell gas turbine systems. At present, this model is not fully implemented into the workbench.

<u>Stack Module</u>. For completeness, the workbench includes a stack. At present, the stack module does not contain any models. However, models could be included to predict items such as aerosol formation, stack opacity or particulate dispersion in the local environment.



Results and Discussion

During the last quarter we have continued development of the CFD models for the entrained flow gasifiers and have performed overall plant simulations using the Vision 21 Workbench. Details are provided below.

Vision 21 Workbench Calculations

To highlight the capabilities of the workbench, a set of four system simulations have been performed for the Vision 21 reference configuration shown in Figure 2. The simulations included the two gasifier types (two stage .vs. one stage) and two fuels (Illinois #6 .vs. Petcoke).

The corresponding Vision 21 network of modules used to perform the simulations is shown in Figure 4. This simulation diagram is an exact representation of the reference diagram with the exception of:

- Hot gas cleanup – while the reference configuration makes use of hot gas cleanup, we have chosen to use warm gas cleanup for our initial testing. To accomplish this, we relocated the heat exchanger, which is normally located downstream of gas cleanup equipment, to upstream of the cleanup equipment. This also eliminated compressed cooling air to the desulfurization unit.
- Gasifier recycle – in the reference configuration, a flue gas recycle stream is pulled following the gas cleanup equipment and fed back to the gasifier. To simplify our initial testing, this recycle stream is currently not considered.
- Gasifier inlet slurry was given exactly as provided via the 0D Gasifier model.
- The air supply stream to the high-pressure fuel cell from the recuperative heater's outlet constitutes a feedback loop, which was eliminated to simplify initial testing. This feedback was simulated by manual iteration of the entire plant until convergence.
- Sulfuric acid plant was not modeled.

For "baseline" gasifier conditions we have used the information provided by DOE (e.g., Table 1, 2 and Figure 2). For the "baseline" we assume the gasifier is a two stage, oxygen blown gasifier operating at 18 atm. and firing (nominally) 3000 tpd Illinois #6 coal. The "baseline" slurry feed is assumed to be 66% solids by weight (dry basis). The slurry temperature is assumed to be 422K and the oxidant temperature is assumed to be 452.5K. The oxidant feed rate is assumed to be 2200 tpd (oxidant =95% O_2 , 5% N_2). Note that we do not have access to the models (or details on calculations) used by DOE to determine the values indicated in Table 2 and Figure 2. In the results discussion below, we assume that the results for using a two stage gasifier firing Illinois #6 (labeled 2 Stage, Illinois #6) is representative of the DOE "baseline" conditions.

Using the 0D gasifier model described in the section for Task 3.3 above, process conditions were created for the other simulations. For the one stage gasifier firing Illinois #6, it was assumed that the coal flow rate and slurry loading should be the same as used in the two stage gasifier simulations. However, operating a one stage gasifier in this manner would result in too low of a bulk gas temperature and lead to slagging problems. Hence, the oxidant flow rate was increased slightly (to ~2400 tpd) to obtain a gas temperature in the gasifier of 2500F, as determined with the 0D model. Due to the much higher heating value of Petcoke the fuel feed rate must be reduced for both gasifiers. In addition, the solids loading in the slurry feed is typically less with Petcoke as compare to coal. Here we have assumed a solids loading of ~56% (dry basis) for the

Petcoke simulations. The 0D gasifier model was used to define the process conditions for firing with Petcoke, subject to the constraint that the gasifier temperature should be the same as for firing with coal.

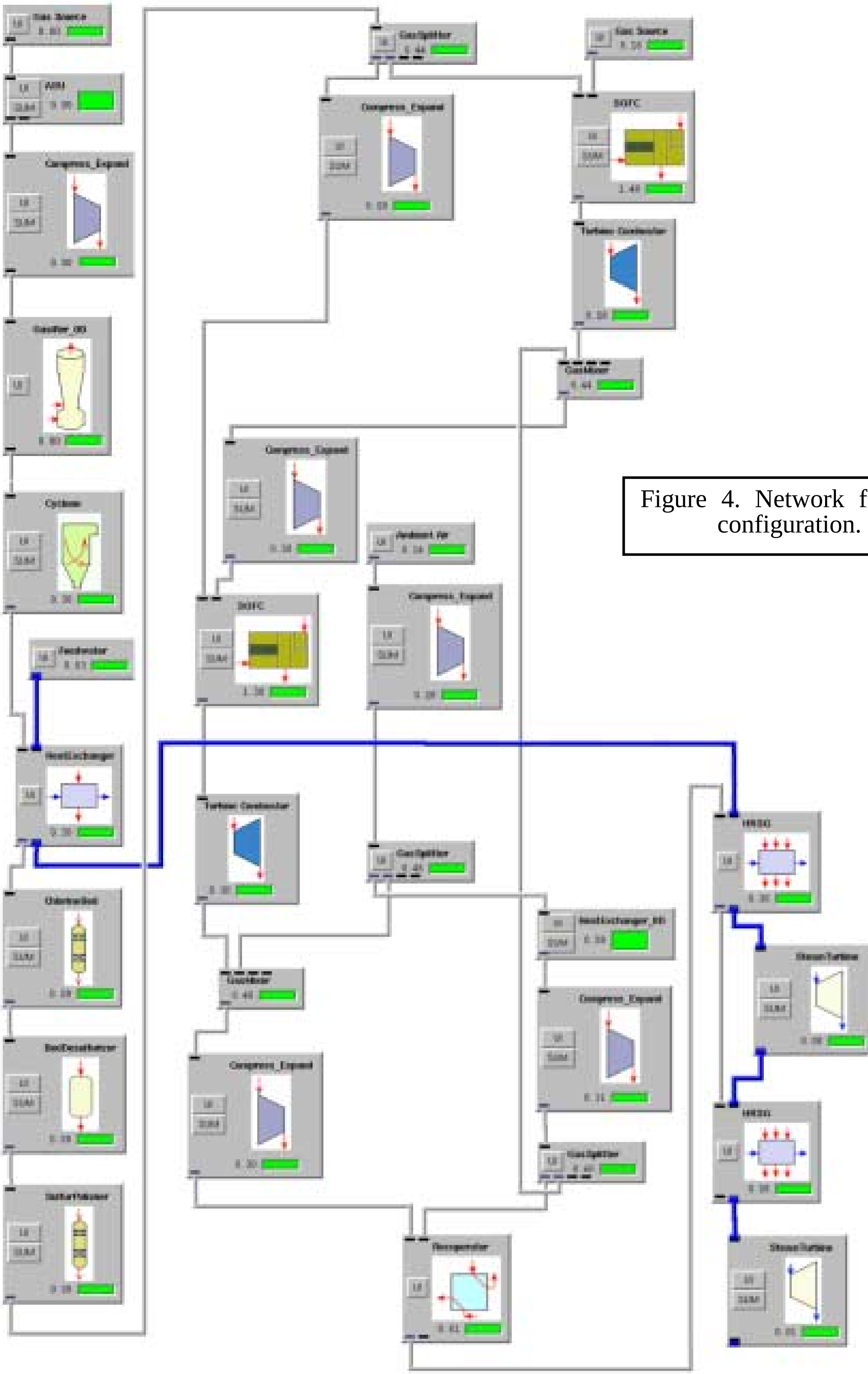


Figure 4. Network for Vision 21 configuration.

Summarized in Tables 3 and 4, respectively, are the fuel properties and process conditions used for the workbench simulations.

Table 3. Fuel Properties

	Illinois #6	Petcoke
Proximate Analysis	As-Received (wt%)	As-Received (wt%)
Moisture	11.12	7.00
Ash	9.70	0.48
Volatile Matter	34.99	12.40
Fixed Carbon	44.19	80.12
TOTAL	100.00	100.00
HHV (Btu/lb)	11666	14282
Ultimate Analysis	As-Received (wt%)	As-Received (wt%)
Moisture	11.12	7.00
Carbon	63.75	81.37
Hydrogen	4.50	2.55
Nitrogen	1.25	0.92
Sulfur	2.80	4.81
Ash	9.70	0.48
Oxygen (by difference)	6.88	2.87
TOTAL	100.00	100.00

Table 4. Gasifier Process Conditions

Item	2 Stage Ill. #6	2 Stage Petcoke	1 Stage Ill. #6	1 Stage Petcoke
Fuel Flow Rate (tpd)	3000	2500	3000	2520
Slurry – wt % (dry basis)	66 %	56%	66 %	56%
Oxidant Flow Rate (tpd)	2200	1940	2400	2140
Slurry Temperature (K)	422	422	422	422
Oxidant Temperature (K)	452	452	452	452

For equipment other than the gasifier, inputs for the associated component model were taken directly from the reference configuration. In cases where data was not provided, data from similar units was used or the component was configured to obtain the proper results for the "baseline" simulation. The inputs for these components were not changed for subsequent simulations. As a result, some downstream equipment might not be configured to operate in an optimal manner for the non-baseline simulations.

Results – Workbench Simulations

Illustrated in Figure 5a-b are the results of the workbench simulations. Shown in Figure 5a is the predicted overall plant efficiency. Illustrated in Figure 5b is the predicted Net Power for the principal power producing components.

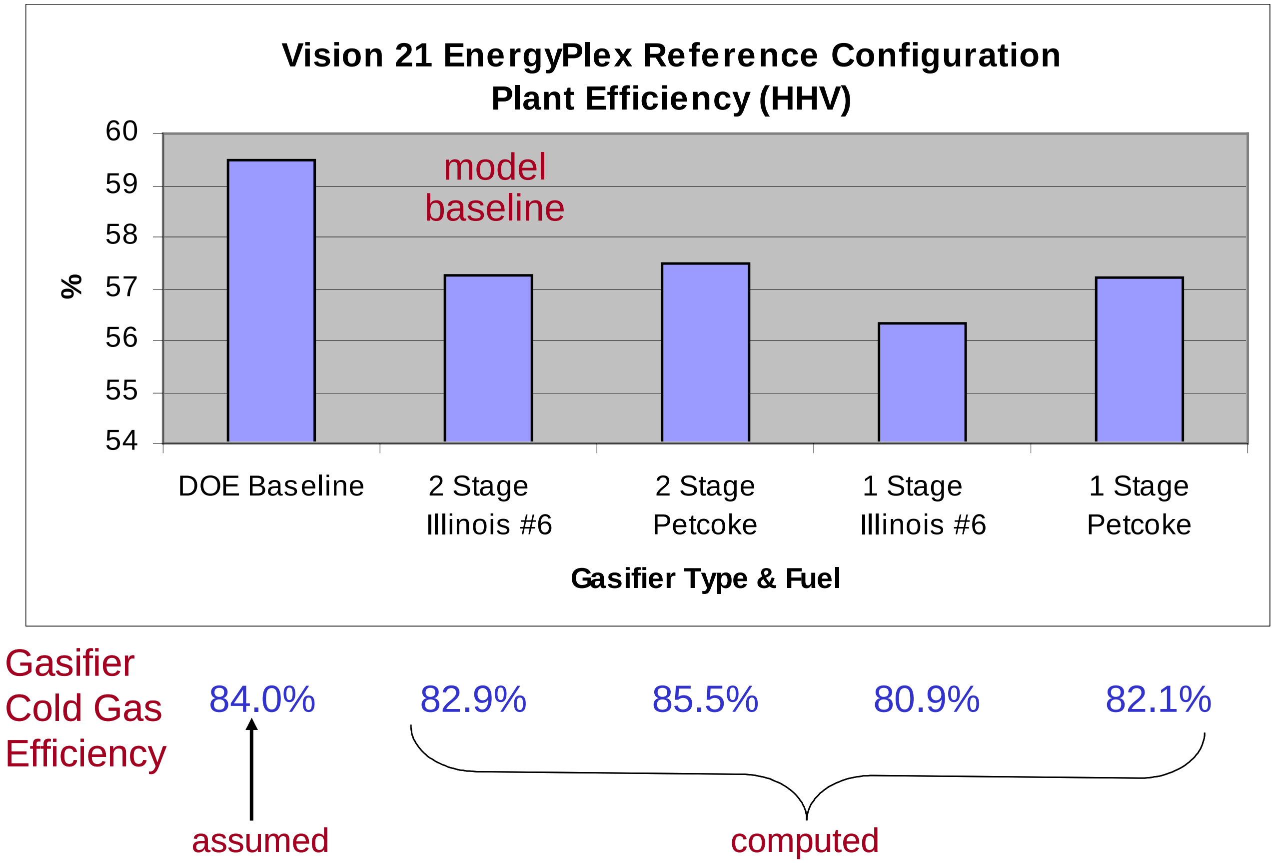


Figure 5a. Vision 21 Workbench Simulation Results – Plant Efficiency.

Several items can be seen from the plots in Figures 5a. Although the overall plant efficiency is slightly less for the simulations as compared to the DOE values, there is remarkably good agreement between the two – despite having to make many assumptions about model inputs, equipment, etc. The DOE overall plant efficiency is 59.5%, which is only slightly less than the Vision21 target value of 60%. As expected, the plant efficiency is slightly higher for the two stage as opposed to the one stage gasifier and the plant efficiency increases when firing Petcoke.

It should be noted that the Gasifier Cold Gas Efficiency shown in Figure 5a and 5b is a computed value for the workbench simulations but an *assumed* value in the DOE information. The computed cold gas efficiency for the models appears to have the expected trend: the two stage gasifier has a higher cold gas efficiency than the one stage gasifier and the cold gas efficiency increases with either gasifier when firing Petcoke.

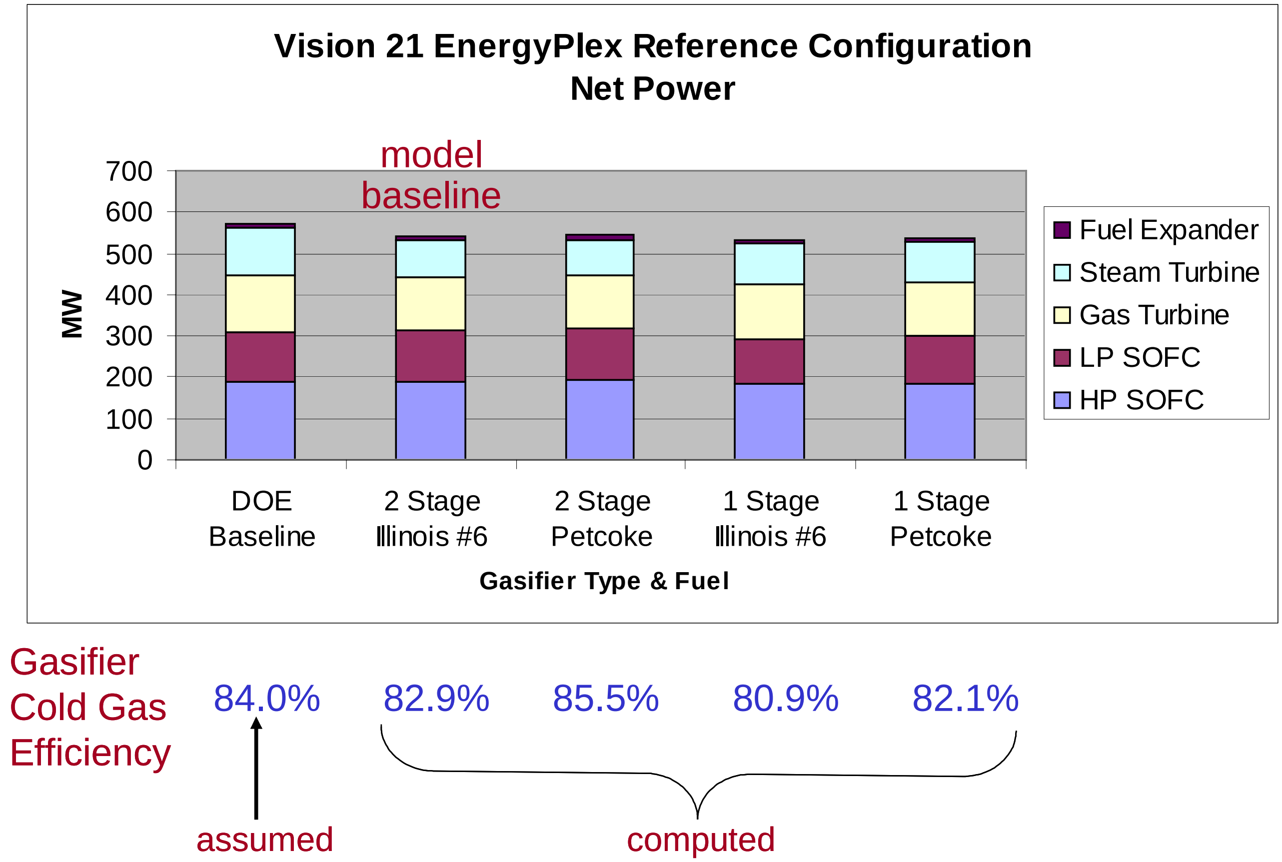


Figure 5b. Vision 21 Workbench Simulation Results – Net Power generated by main components.

Comparing the Net Power results in Figure 5b, again there is good agreement between DOE provided values and the workbench calculated values. Comparing the DOE and computed net power for the fuel cell there appears to be very good agreement. However, there does appear to be a noticeable difference between the DOE and computed net power values at the steam turbine. This is likely due to the relatively simple HSRG model used in our workbench due to the lack of detail provided within the reference configuration

As discussed above, the baseline process conditions for the two stage gasifier were determined using the coal, oxidant and slurry flow rates as specified by DOE. As a result the Cold Gas Efficiency of the gasifier model did not agree with the DOE value of 84%. A potential future study would be to alter the gasifier process conditions and possibly the gasifier geometry (i.e., residence time) to match the assumed DOE gasifier cold gas efficiency of 84%, and to then repeat the overall workbench simulations.

In the following two sections we briefly summarize some CFD simulations for the one stage and two stage gasifier that were performed as part of the workbench simulations discussed above.

Results – Two Stage CFD Gasifier Model

The gross gasifier geometry used for these simulations is summarized in Figure 6. The process conditions are based on the Vision 21 reference configuration and have been described above. The flow distributions by injector level are the same as used in previous simulations of this gasifier [Bockelie et al, 2002c,d,e]: all of the oxidant and 78% of the coal is uniformly distributed amongst the fuel injectors in the first stage and the remaining coal is uniformly distributed across the injectors in the second stage. No oxidant is injected into the upper stage. For firing the Illinois #6 coal, the overall oxygen:carbon (O_2:C) mole ratio is ~0.40, resulting in an overall stoichiomery of about ~0.48 and a stoichiometry in the lower stage of about ~0.62. However for firing Petcoke, the overall oxygen:carbon (O_2:C) mole ratio is ~0.34, resulting in an overall stoichiomery of about 0.47 and a stoichiometry in the lower stage of about 0.60.

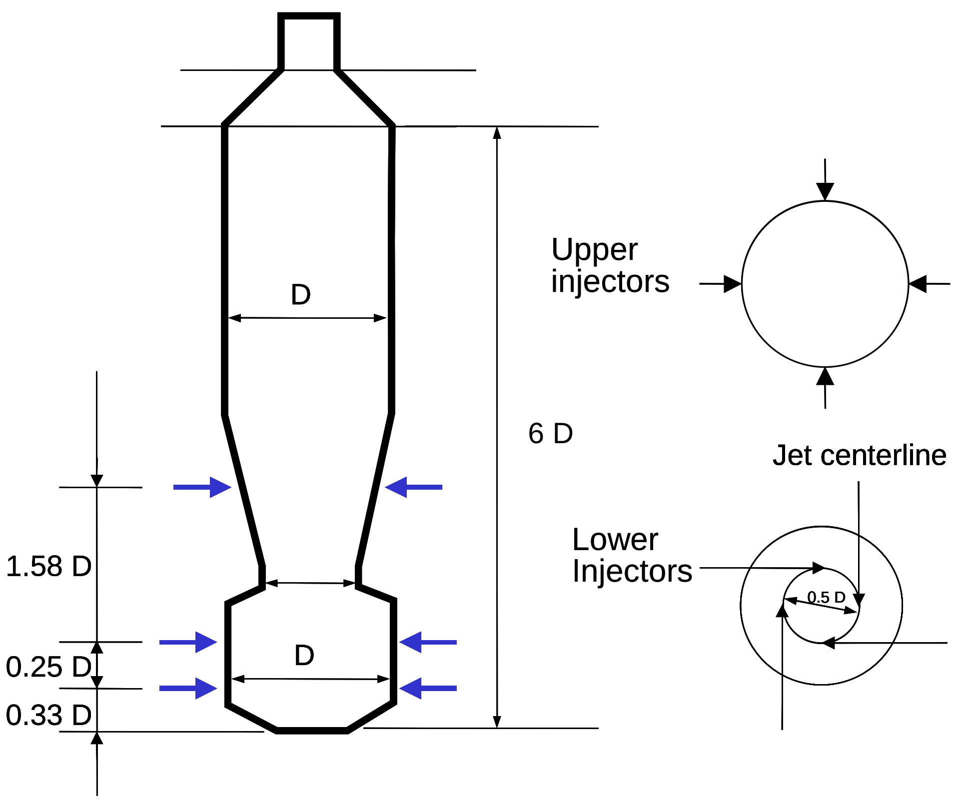


Figure 6. Schematic of Two-Stage Up Flow configuration.

Illustrated in Figures 7 and 8 are the gross flow fields for the two-stage gasifier for the prescribed operating conditions firing Illinois #6 and Petcoke, respectively. To simplify plotting, only the bottom portion of the gasifier is included in the figures. Shown in Figure 7 are the predicted gas temperature and H2 and CO gas species concentration (volume %) at selected elevations. Also shown in Figure 7 are representative coal particle trajectories colored by coal volatile content and coal char content. Figure 8 contains the same plots but for firing Petcoke instead of Illinois #6.

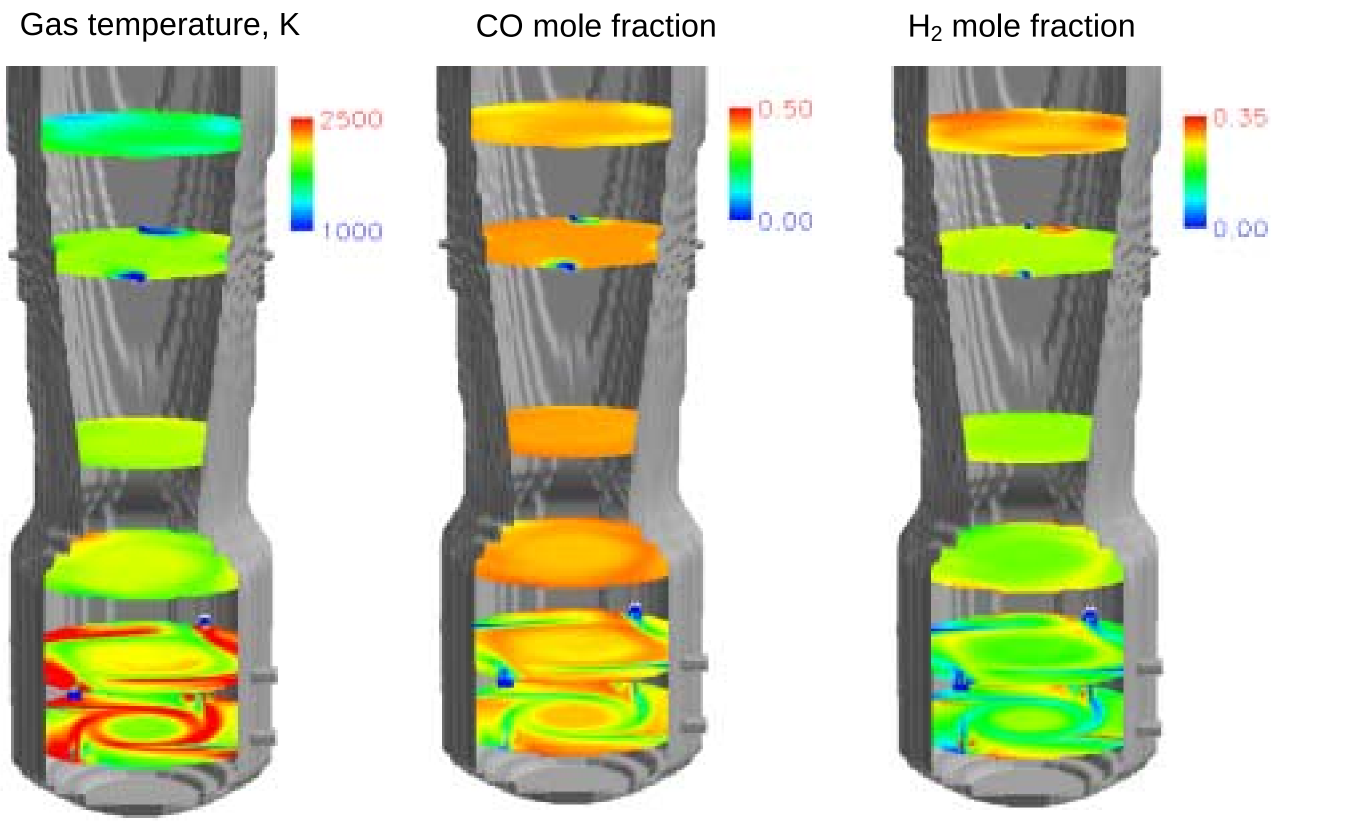
From the figures one can see a strong, swirling flow pattern in the gas flow and the particle trajectories in the lower section. This pattern is to be expected with a tangential firing system used for the lower injectors. Looking at the flow field immediately in front of the top level of injectors the flow pattern changes due to these injectors being oriented opposed to each other. As illustrated by the fuel particle trajectories shown in Figure 7, the fuel injected into the first stage devolatilizes very quickly but the fuel injected at the top injectors requires a slightly longer time to devolatilize. The char from fuel injected in the first stage almost completely gasifies prior to reaching the upper injectors. However, the char in the fuel particles from the upper injectors requires a very long time to fully gasify.

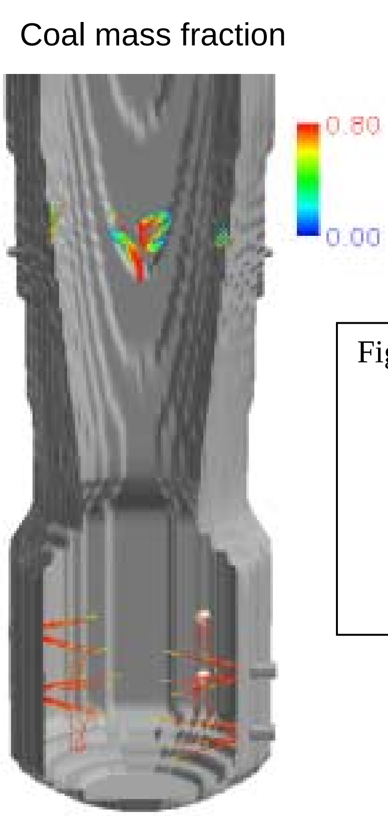
Comparing the flow fields for firing Illinois #6 versus Petcoke it is difficult to identify significant differences. However, this should not be surprising because the gasifier operating conditions for firing Petcoke were designed to provide a comparable gasifier temperature as for firing Illinois #6.

Listed in Table 5 are gross gasifier exit values from the CFD simulation for firing Illinois #6 and Petcoke. Here slight differences in the gasifier performance can be seen, most notably in the exit CO concentration and the predicted LOI for the unburned fuel exiting the gasifier and deposited on the walls.

Table 5. Two Stage Gasifier Results.

	Illinois#6	Petcoke
Exit Temperature, K	1412	1406
Carbon Conversion, %	91.4	93.9
Exit LOI, %	34.2	76.7
Deposit LOI, %	47.9	96.4
Deposition, %	8.5	4.7
PFR Residence Time, s	0.83	0.83
Particle Residence Time, s	0.37	0.19
Mole Fraction: CO	43.3%	47.3%
H_2	32.7%	31.4%
H_2O	13.3%	11.0%
CO_2	8.1%	7.6%
H_2S	0.8%	1.2%
COS	0.0%	0.1%
N_2	1.6%	1.3%
Exit Mass Flow, klb/hr	497	507
HHV of Syngas, Btu/lb	4988	5050
HHV of Syngas, Btu/SCF	248	257
Cold-Gas Efficiency, %	82.9	85.5





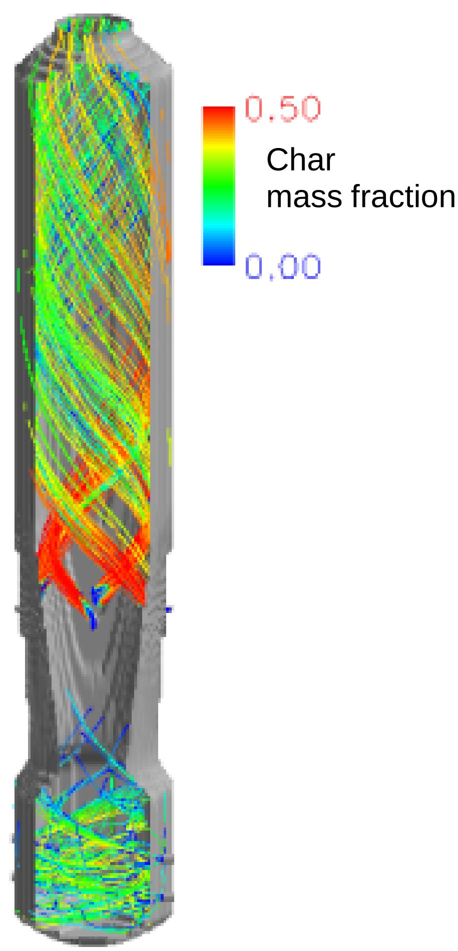
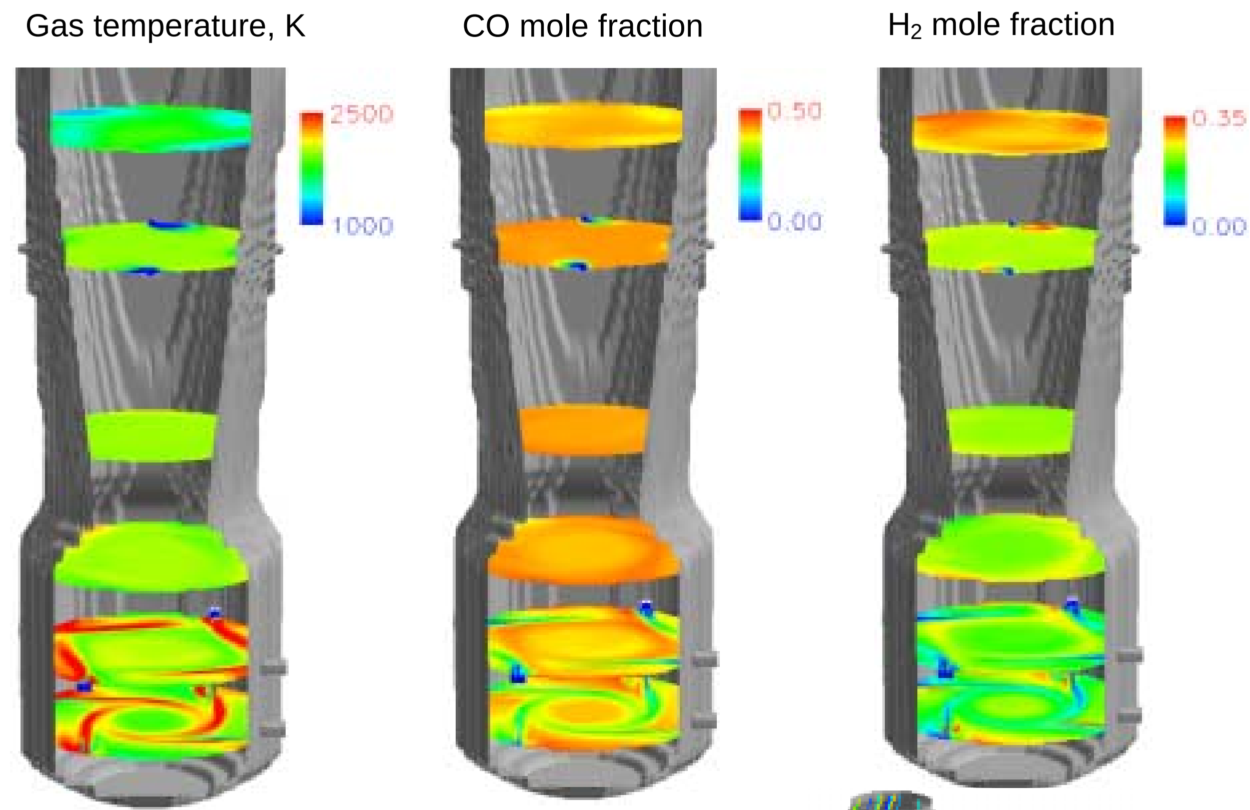
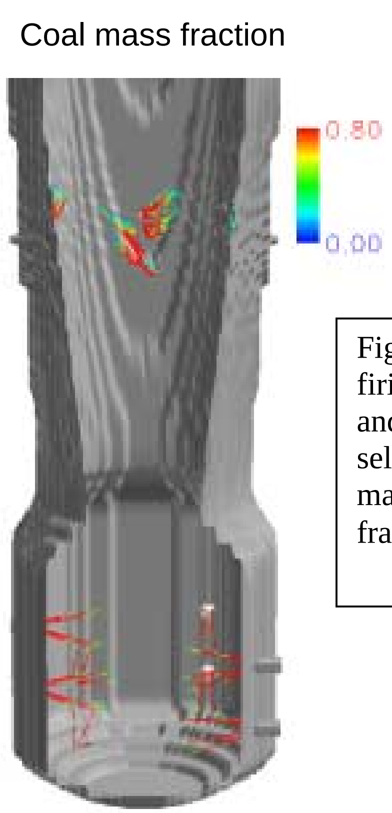


Figure 7. Two-stage gasifier firing **Illinois #6**. Shown are gas temperature, CO and H2 concentration at selected elevations Coal mass fraction and char mass fraction for selected trajectories.





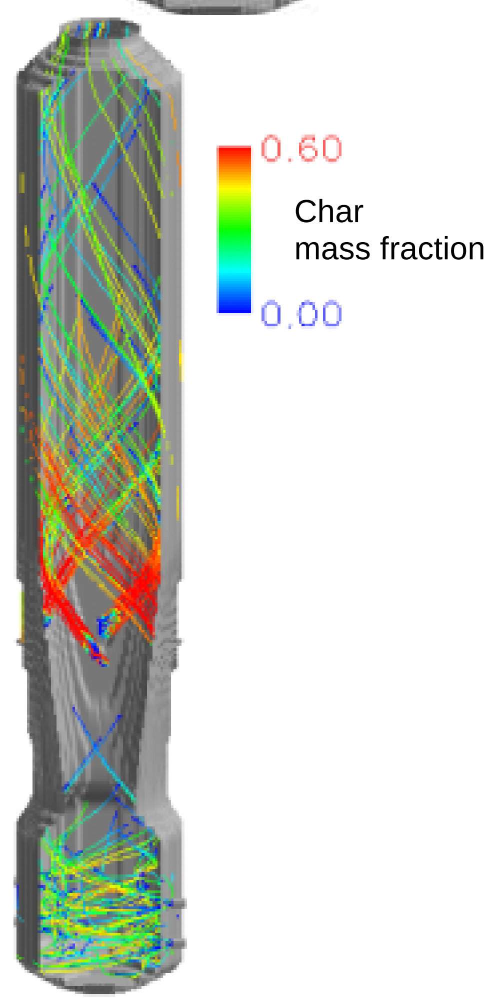


Figure 8. Two Stage Gasifier firing Petcoke. Gas temperature and gas concentration at selected elevations and coal mass fraction and char mass fraction for selected trajectories.

Results - Single Stage CFD Gasifier Model

The process conditions are summarized above in the discussion on the Vision 21 workbench calculations and the gasifier geometry is highlighted in Figure 9. The general assumptions about the gasifier operation are the same as used in previous simulations for this gasifier [Bockelie et al, 2002c,d,e].

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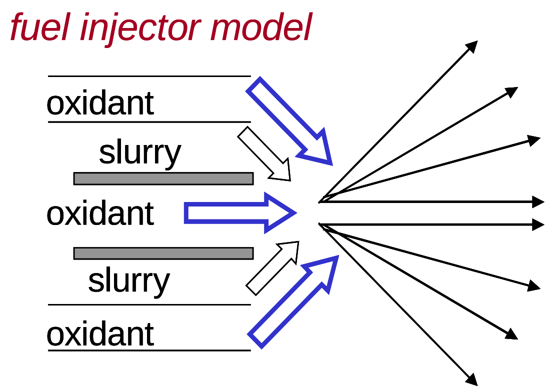

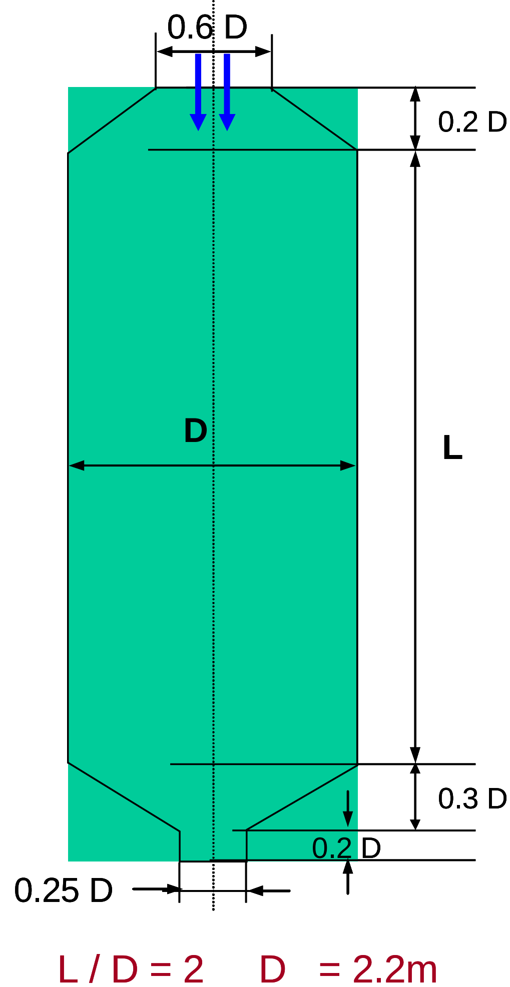

Figure 9. Schematic of One-Stage DownFlow gasifier.

Illustrated in Figures 10 and 11 are the gasifier gross flow fields for a single stage firing Illinois #6 and Petcoke, respectively. Shown in Figure 10 are the predicted gas temperature and CO and H2 species concentration (volume %) at mid-plane of the gasifier. Figure 11 contains the same plots as Figure 10, but for firing Petcoke instead of Illinois #6.

Overall, the gross flow field is similar to that of an immersed jet exhausting into a confined volume. There is a core of high velocity, hot gas traveling down the center of the gasifier. Away from the centerline, there exists a slow moving, much cooler reversed flow (i.e., recirculating flow) that travels back toward the injector end of the gasifier.

Comparing the flow field for firing Illinois #6 versus that of firing Petcoke the only noticeable difference is for the CO concentration. Listed in Table 6 is a comparison of average values for the one stage gasifier simulations. Again, there are not significant differences.

If one compares the gasifier exit conditions for the one stage versus those of the two stage, the most notable difference is in gas exit temperature (which is also reflected in the Cold Gas Efficiency values). Also, the H2 and H2O concentrations at the gasifier exit are somewhat different between the two gasifier process conditions.

Table 6. One Stage Gasifier Results.

	Illinois#6	Petcoke
Exit Temperature, K	1595	1669
Carbon Conversion, %	92.2	89.1
Exit LOI, %	22.4	79.6
Deposit LOI, %	53.1	97.9
Deposition, %	8.5	9.0
PFR Residence Time, s	0.80	0.78
Particle Residence Time, s	0.16	0.12
Mole Fraction: CO	43.4%	47.2%
H_2	29.7%	28.0%
H_2O	16.3%	14.6%
CO_2	8.1%	7.6%
H_2S	0.8%	1.1%
COS	0.0%	0.1%
N_2	1.7%	1.4%
Exit Mass Flow, klb/hr	517	522
HHV of Syngas, Btu/lb	4671	4674
HHV of Syngas, Btu/SCF	241	246
Cold-Gas Efficiency, %	80.9	82.1

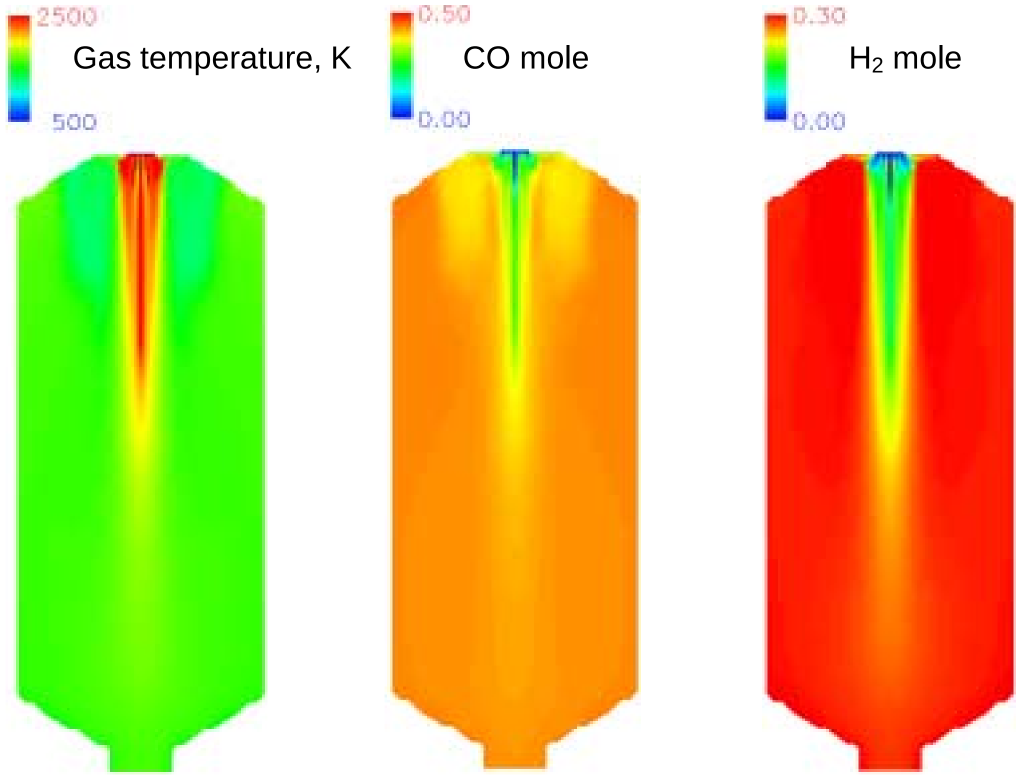

Figure 10. One Stage Gasifier firing Illinois #6. Gas Temperature, CO and H2 species concentrations at selected planes.

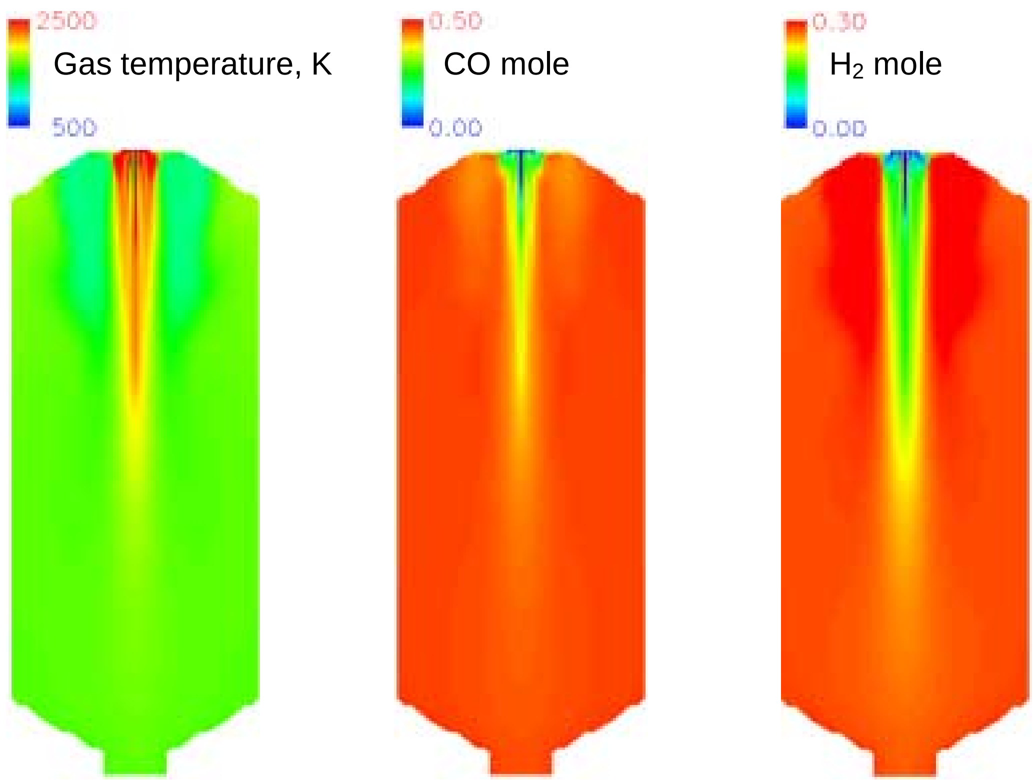

Figure 11. One Stage Gasifier firing Petcoke. Gas Temperature, CO and H2 species concentrations at selected planes.

Flowing Slag Model - Single Stage Up Fired Gasifier

Additional simulations have been performed for a single stage up fired, dry feed gasifier. The purpose in revisiting these simulations was to eliminate some visible flowfield asymmetries that occurred in the lower section of the gasifier [Bockelie et al, 2002c,d]. This gasifier has been used to build confidence in the flowing slag model that has been implemented into the CFD gasifier model. These simulations were not performed as part of the Vision 21 Workbench calculations.

The gasifier uses a water jacket to cool the refractory. The backside cooling results in a "solid" slag layer on the refractory hot side that protects the refractory from the harsh conditions within the gasifier. The configuration is representative of the Prenflo gasifier being used at the IGCC plant at Puertellano, Spain. Our interest in this configuration is the availability of flowing slag model results that have been published by other researchers [Seggiani, 1998], [Benyon, 2002].

Illustrated in Figure 12 are representative values for the flow field in the gasifier. The gasifier is assumed to be fired with 2600 tpd of dried bituminous coal, employs a dry feed system (nitrogen is used for the solids transport gas) and the oxidant flow rate results in an inlet stoichiometry of about 0.4. It is assumed that no gas exits through the slag tap at the bottom of the reactor and thus all flue gas must exit through the top. Detailed descriptions of the gasifier geometry and process conditions are available in [Seggiani, 1998], and [Bockelie et al, 2002d] and thus are not repeated here.

As can be seen from Figure 12, the firing system consists of four fuel injectors in a diametrically opposed pattern located near the bottom of the gasifier. In addition, it can be seen that the bulk of the chemical reactions occur in narrow band at the fuel injector elevation. As expected, the flow field in the lower region of the gasifier is roughly symmetric in 90 degree sections.

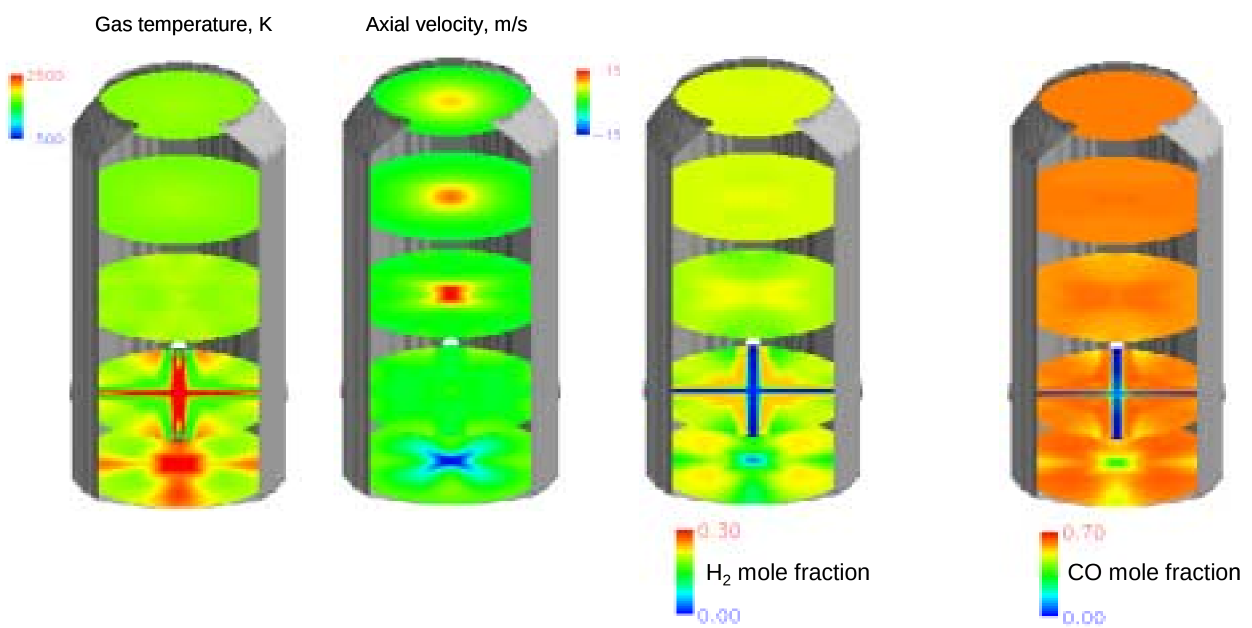

Figure 12. Gas temperature, axial velocity and H2 and CO concentration (mole fraction).

The table at right lists the gasifier performance in terms of syngas exit conditions for the simulations conducted by Seggiani, Benyon and our model (REI). Overall there is good agreement between the three models. Note that table entries in parentheses [ ] indicate values from the other researchers that we have estimated based on their published values. Similarly, table entries with a dash (-) indicate items for which data is not listed in the reports from the other studies. In the report by Seggiani, it is stated that the design conditions for this gasifier call for ~99% carbon conversion. It should be noted that the gasifier model used in our study has substantially more mesh resolution than used by the other researchers. The model developed by Seggiani was a 1D zonal model consisting of ~15 zones and the model by Benyon was a 3D CFD model that used ~10K cells to model a 90 degree section of the gasifier. The model used in this study contains ~400K cells.

Exit conditions	Seggiani	Benyon	REI
Gas temp, K	1803	[1650]	1790
CO (wt%)	76.5	70.9	76.8
CO_2 (wt%)	3.2	10.0	6.0
H_2 (wt%)	1.8	1.8	1.9
H_2O (wt%)	-	-	3.2
N_2 (wt%)	-	-	10.1
Deposition (%)	-	-	4.7
Carbon conversion (%)	-	-	99.99
HHV, Btu/lb	[4431]	[4248]	4622
Cold-gas efficiency (%)	-	[91.5]	80.5

Illustrated in Figure 13 are plots that compare the slag model values predicted by Seggiani, Benyon and our model (REI). Plotted as a function of gasifier elevation is the average value for:

- liquid (molten) slag thickness,
- “frozen” or solid slag thickness,
- slag surface temperature (i.e., surface temperature “seen” by the gas field), and
- net heat flux to the liquid slag surface (wall heat flux).

Overall, the three models qualitatively predict the same trends and about the same magnitudes. The model results predict a liquid slag thickness of a few millimeters and a solid slag thickness that varies between 10-20 mm. (<1 inch). Annomalies in the slag properties can be seen at the fuel injector elevation (~2m.) and near the slag tap (~0m.). Based on the coal and flux material properties in [Seggiani, 1998], the critical viscosity should be about 1625K, which the model predicts to be achieved, implying that a solid slag layer should exist. In addition, our slag model results indicate very high gas temperatures near the bottom of the gasifier, resulting in a high heat flux and thus potentially creating a situation where it is too hot for solid slag to exist on the bottom face of the gasifier.

Illustrated in Figure 14 is a more detailed representation of our predicted flowing slag model results. Here, we have mapped the local values from the slag model to a 2D representation of the inner surface of the gasifier. The figure is created, in effect, by “painting” the inside surface of the gasifier with the predicted values and then plotted by projecting these values onto a flat, 2D plane. With this representation the local variations in the predicted values can be visualized. The color map for the different plots is included in Figure 14 (in general, dark blue is a low value and red is a high value). From the plots it can be seen that the predicted slag thickness, surface temperature and wall heat flux do not change significantly in the circumferential direction except for near the fuel injectors where a noticeable anomaly in values occurs. As per the gasifier flowfield, the predicted slagging properties in the present simulations are far more symmetric in appearance than the previously reported values [Bockelie et al, 2002d].

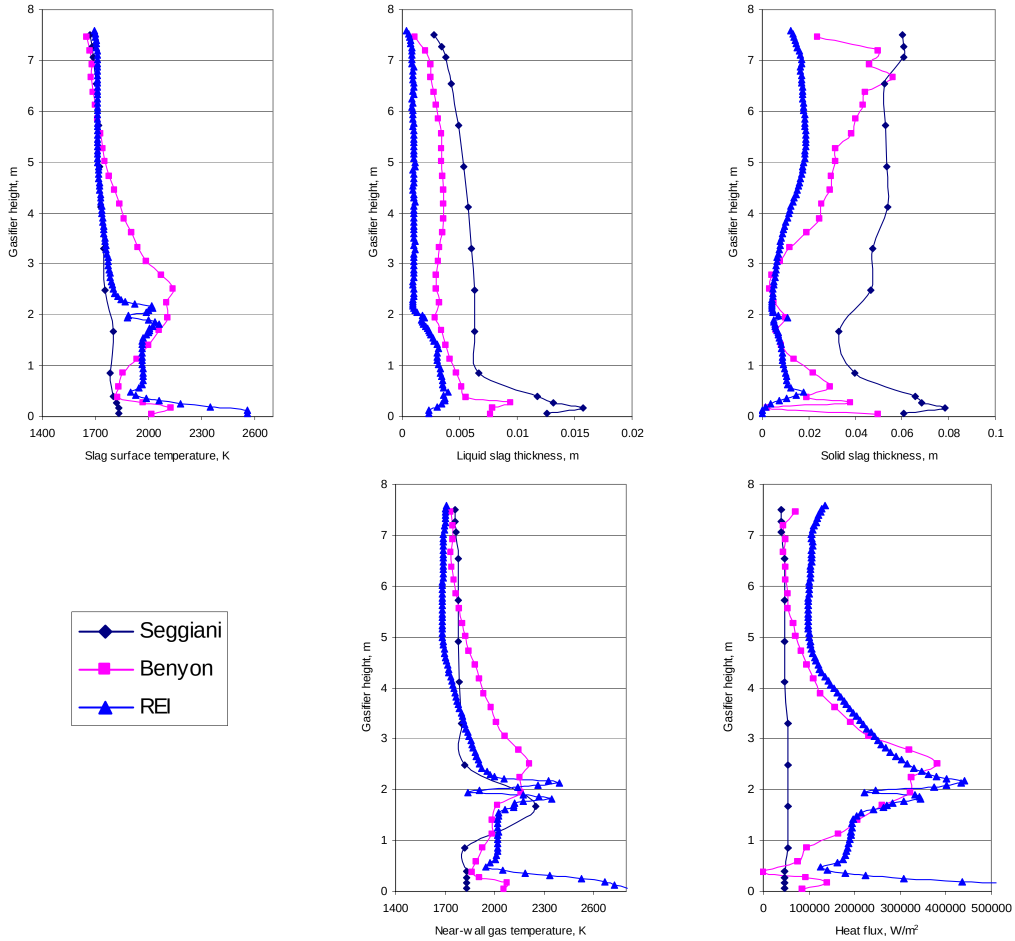

Figure 13. Comparison of flowing slag model

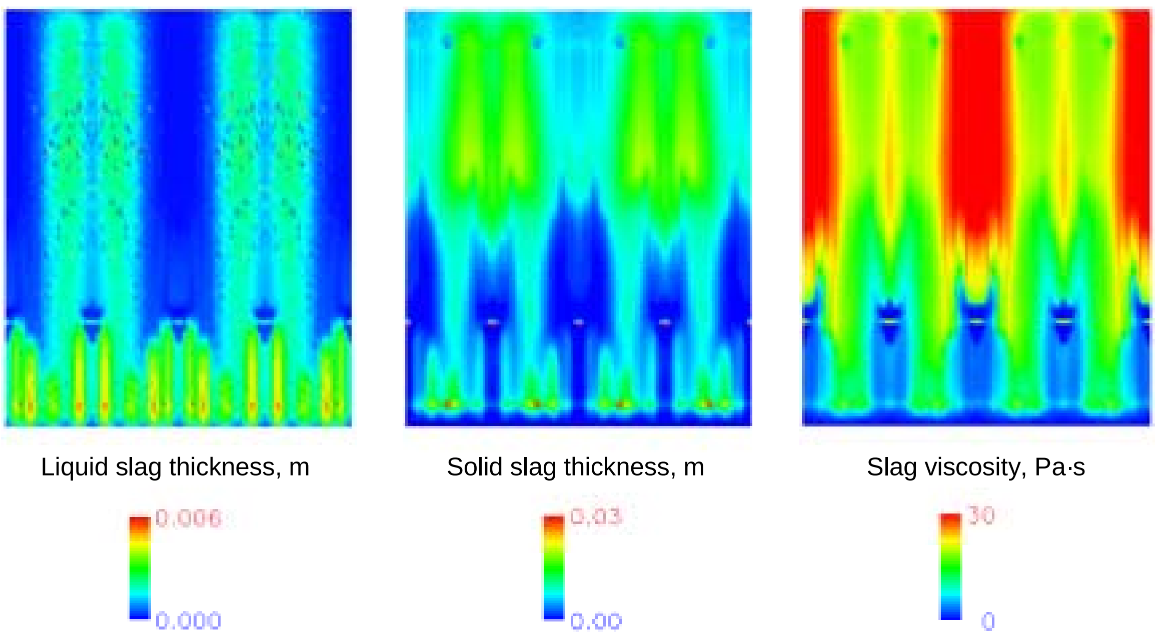

Figure 14. Predicted slag model results displayed as 2D plots.

Preliminary Gasifier Calculations - *AIOLOS*

The work during the last performance period has been focused on the definition of a two-stage industrial gasifier configuration, and on the generation of steady state results for this configuration. A geometry model for the following configuration has been set up:

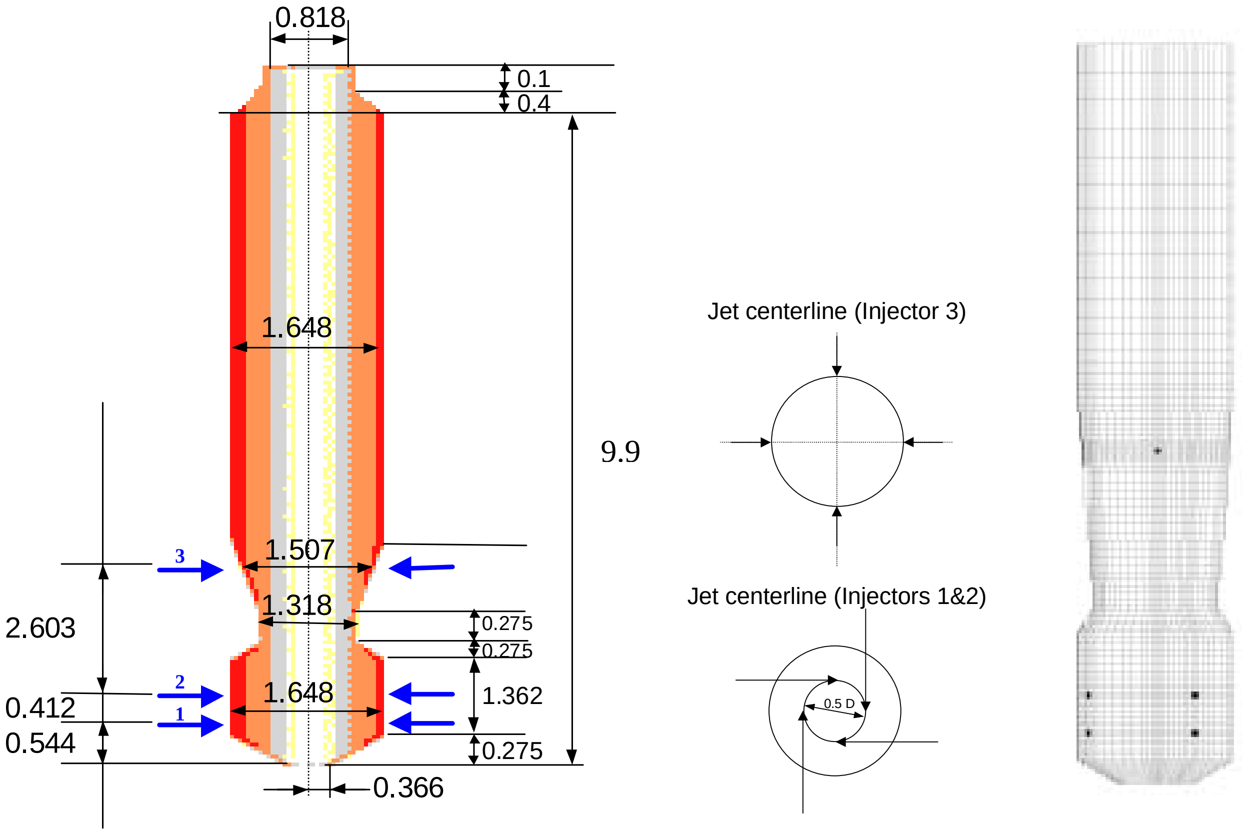

Figure 15. Two Stage Industrial Gasifier Configuration (Left) and Geometry Model (Right)

The geometry model does only cover the lower part (up to a height of 8 m) of the entire gasifier geometry.

Steady state results have been generated for the following operating conditions using an Illinois coal #6 (see Table 2) with a uniform size 39.8 µm as the base fuel:

Coal flow rate:	32.274 kg/s
O_2 (95% vol.) and N_2 (5% vol.) flow rate:	23.128 kg/s
H_2O (for wet slurry) flow rate:	11.188 kg/s
Gasifier pressure:	18 atm
Inlet coal temperature:	422 K
Inlet O_2 temperature:	475 K

Steady state results have been generated assuming a completely dried coal with 100 % vaporized slurry water. Furthermore, the injectors have been modeled assuming ideal mixing between the streams. The results achieved using the gasification chemistry model implemented in the present project are shown in Figure 16 and 17. Figure 16 and 17 show average profiles of major species concentrations, and average temperature over gasifier height. The predicted gasifier exit conditions are summarized in Table 7.

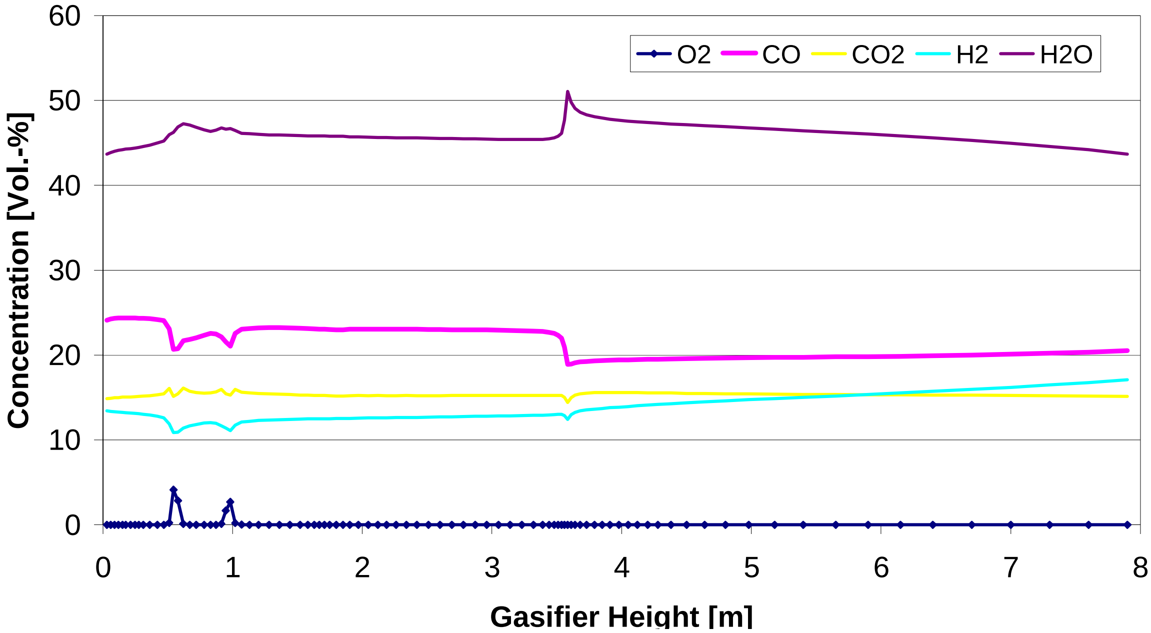

Figure 16: Average profiles of major species concentrations over gasifier height.

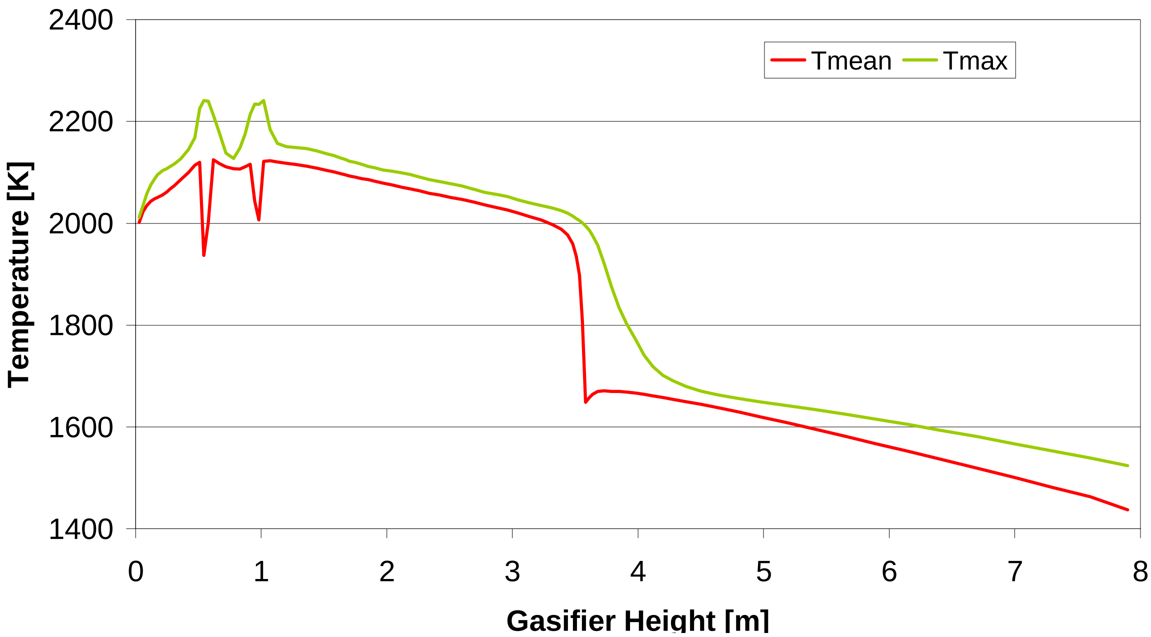

Figure 17: Profiles of average and peak temperature over gasifier height.

Table 7: Predicted 2-stage gasifier exit conditions

CO-Concentration	20.5 Vol.-%
H2-Concentration	17.1 Vol.-%
H2O-Concentration	43.7 Vol.-%
CO2-Concentration	15.0 Vol.-%
CH4-Concentration	0.23 Vol.-%
O2-Concentration	0.00 Vol.-%
Heating Value and Mass Flow	7,330 kJ/kgGas(62.85 kgGas/s)
Cold Gas Efficiency	52,6 %

The analysis of the steady state profiles indicate that the gasification process is not completed at the height of 8m, which was chosen to minimize the computational effort and improve the response time for the subsequent transient runs that are planned during the project. This explains the low cold gas efficiency and heating value at the exit of the computational domain. Therefore, a further extension of the model will be done to identify, where the gasification process reaches the final composition.

Conclusions

During the last quarter good progress has been made on the development of an IGCC workbench. A fully functional Vision 21 workbench is available for use. A full complement of models has been implemented into the workbench and preliminary process simulations have been performed.

Calculations for a full Vision 21 plant configuration have been performed for two coal types and two gasifier types. Good agreement with DOE computed values has been obtained for the Vision 21 configuration under "baseline" conditions. Additional model verification has been performed for the flowing slag model that has been implemented into the CFD based gasifier model. Comparisons for the slag, wall and syngas conditions predicted by our model versus values from predictive models that have been published by other researchers show good agreement. The software infrastructure of the IGCC workbench has been modified to use a recently released, upgraded version of SCIRun. Exploratory work has been performed for developing a standardized CCA model interface, tailored to Vision 21, using the SIDL interface definition language.

Plans for the next quarter include: additional simulations to explore and exercise the capabilities of the full Vision 21 workbench; parametric studies with the 0D zonal gasifier model to build confidence in the values predicted; further development of the CFD gasifier models, with special focus on reaction kinetics, the slagging wall model and additional parametric cases; and continued investigation and testing of component architectures and interface standards (CCA, CORBA, CAPE-Open) and their use for our Vision 21 workbench.

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